finufft Documentation

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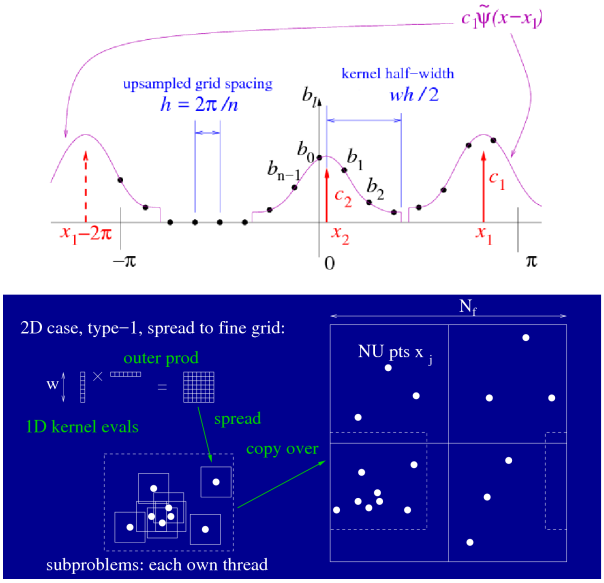

FINUFFT is a set of libraries to compute efficiently three types of nonuniform fast Fourier transform (NUFFT) to a specified precision, in one, two, or three dimensions, on a multi-core shared-memory machine. The library has a very simple interface, does not need any precomputation step, is written in C++ (using OpenMP and FFTW), and has wrappers to C, fortran, MATLAB, octave, and python. As an example, given M arbitrary real numbers x_j and complex numbers c_j, with $j = 1, \ldots, M$, and a requested integer number of modes N, the 1D type-1 (aka "adjoint") transform evaluates the N numbers

$$f_k = \sum_{j=1}^{M} c_j e^{ikx_j} \ , \qquad \text{for } \ k \in \mathbb{Z}, \quad -N/2 \le k \le N/2 - 1 \ . \tag{1}$$

The x_j can be interpreted as nonuniform source locations, c_j as source strengths, and f_k then as the kth Fourier series coefficient of the distribution $f(x) = \sum_{j=1}^{M} c_j \delta(x - x_j)$. Such exponential sums are needed in many applications in science and engineering, including signal processing, imaging, diffraction, and numerical partial differential equations. The naive CPU effort to evaluate (1) is $O(NM)$. The library approximates (1) to a requested relative precision ϵ with nearly linear effort $O(M \log(1/\epsilon) + N \log N)$. Thus the speedup over the naive cost is similar to that achieved by the FFT. This is achieved by spreading onto a regular grid using a carefully chose kernel, followed by an upsampled FFT, then a division (deconvolution) step. For the 2D and 3D definitions, and other types of transform, see below.

The FINUFFT library achieves its speed via several innovations including:

1. The use of a new spreading kernel that is provably close to optimal, yet faster to evaluate than the Kaiser-Bessel kernel
2. Quadrature approximation of the Fourier transform of the spreading kernel
3. Blocked multithreading of the type-1 spreading operation

For the same accuracy in 3D, the library is 2-12 times faster on a single core than the single-threaded fast Gaussian gridding CMCL libraries of Greengard-Lee, and in the multi-core setting is usually faster than the Chemnitz NFFT3 library even when the latter is allowed a RAM-intensive full precomputation of the kernel. This is especially true for highly non-uniform point distributions and/or high precision. Our library does not require precomputation and uses minimal RAM.

CHAPTER

ONE

INSTALLATION

Obtaining FINUFFT

Go to the github page https://github.com/ahbarnett/finufft and follow instructions (eg see the green button).

Dependencies

This library is currently only supported for unix/linux, and partially for Mac OSX. We have heard that it can be compiled on Windows too.

For the basic libraries

- C++ compiler such as `g++` packaged with GCC
- FFTW3
- GNU make

Optional:

- `numdiff` (preferred but not essential; enables pass-fail math validation)
- for Fortran wrappers: compiler such as `gfortran`
- for matlab/octave wrappers: MATLAB, or octave and its development libraries
- for building new matlab/octave wrappers (experts only): `mwrap`
- for the python wrappers you will need `python` and `pip` (if you prefer python v2), or `python3` and `pip3` (for python v3)

Tips for installing dependencies on various operating systems

On a Fedora/CentOS linux system, these dependencies can be installed as follows:

```
sudo yum install make gcc gcc-c++ gcc-gfortran fftw3 fftw3-devel libgomp octave octave-devel
```

then see below for `numdiff` and `mwrap`.

Note: we are not exactly sure how to install python3 and pip3 using yum

then download the latest `numdiff` from http://gnu.mirrors.pair.com/savannah/savannah/numdiff/ and set it up via `./configure; make; sudo make install`

On Ubuntu linux (assuming python3 as opposed to python):

```
sudo apt-get install make build-essential libfftw3-dev gfortran numdiff python3 python3-pip octave li
```

On Mac OSX:

Make sure you have `make` installed, eg via XCode.

Install gcc, for instance using pre-compiled binaries from http://hpc.sourceforge.net/

Install homebrew from http://brew.sh:

```
brew install fftw
```

Install `numdiff` as below.

(Note: we are not exactly sure how to install python3 and pip3 on mac)

Currently in Mac OSX, `make lib` fails to make the shared object library (.so); however the static (.a) library is of reasonable size and works fine.

Installing numdiff

numdiff by Ivano Primi extends `diff` to assess errors in floating-point outputs. Download the latest `numdiff` from the above URL, un-tar the package, cd into it, then build via `./configure; make; sudo make install`

Installing MWrap

MWrap is a very useful MEX interface generator by Dave Bindel. Make sure you have `flex` and `bison` installed. Download version 0.33 or later from http://www.cs.cornell.edu/~bindel/sw/mwrap, un-tar the package, cd into it, then:

```
make
sudo cp mwrap /usr/local/bin/
```

Compilation

Compile and test FINUFFT via:

```
make test
```

or, to compile using all available cores:

```
make test -j
```

This should compile the main libraries then run tests which should report zero crashes and zero fails. (If numdiff was not installed, it instead produces output that you will have to check by eye matches the requested accuracy.) If you have an error then `cp makefile makefile.local`, edit `makefile.local` to adjust compiler and other library options, and use `make -f makefile.local test`. Run `make` without arguments for full list of possible make tasks.

If there is an error in testing on a standard set-up, please file a bug report as a New Issue at https://github.com/ahbarnett/finufft/issues

Building examples and wrappers

`make examples` to compile and run the examples for calling from C++ and from C.

The `examples` and `test` directories are good places to see usage examples.

`make fortran` to compile and run the fortran wrappers and examples.

`make matlab` to build the MEX interface to matlab.

`make octave` to build the MEX-like interface to octave.

Building the python wrappers

First make sure you have python3 and pip3 (or python and pip) installed and that you have already compiled the C++ library (eg via `make lib`). Next make sure you have NumPy installed:

```
pip3 install numpy
```

Then do the following from the main `finufft` install directory:

```
pip3 install .
```

You can then run the tests as follows:

```
cd python_tests
python3 demo1d1.py
python3 run_accuracy_tests.py
python3 run_speed_tests.py
```

In all of the above the "3" can be omitted if you want to work with python v2.

See also Dan Foreman-Mackey's earlier repo that also wraps finufft, and from which we have drawn code: python-finufft

A few words about python environments

There can be confusion and conflicts between various versions of python and installed packages. It is therefore a very good idea to use virtual environments. Here's a simple way to do it (after installing python-virtualenv):

```
Open a terminal
virtualenv -p /usr/bin/python3 env1
. env1/bin/activate
```

Now you are in a virtual environment that starts from scratch. All pip installed packages will go inside the env1 directory. (You can get out of the environment by typing `deactivate`)

CHAPTER

TWO

MATHEMATICAL DEFINITIONS OF TRANSFORMS

We use notation with a general space dimensionality d, which will be 1, 2, or 3, in our library. The arbitrary (ie nonuniform) points in space are denoted $\mathbf{x}_j \in \mathbb{R}^d$, $j = 1, \dots, M$. We will see that for type-1 and type-2, without loss of generality one could restrict to the periodic box $[-\pi, \pi)^d$. For type-1 and type-3, each such NU point carries a given associated strength $c_j \in \mathbb{C}$. Type-1 and type-2 involve the Fourier "modes" (Fourier series coefficients) with integer indices lying in the set

$$K = K_{N_1,\dots,N_d} := K_{N_1} K_{N_2} \dots K_{N_d} \ ,$$

where

$$K_{N_i} := \begin{cases} \{-N_i/2, \dots, N_i/2 - 1\}, & N_i \text{ even}, \\ \{-(N_i-1)/2, \dots, (N_i-1)/2\}, & N_i \text{ odd}. \end{cases}$$

For instance, $K_{10} = \{-5, -4, \dots, 4\}$, whereas $K_{11} = \{-5, -4, \dots, 5\}$. Thus, in the 1D case K is an interval containing N_1 integer indices, in 2D it is a rectangle of $N_1 N_2$ index pairs, and in 3D it is a cuboid of $N_1 N_2 N_3$ index triplets.

Then the type-1 (nonuniform to uniform, aka "adjoint") NUFFT evaluates

$$f_{\mathbf{k}} := \sum_{j=1}^{M} c_j e^{\pm i \mathbf{k} \cdot \mathbf{x}_j} \qquad \text{for } \mathbf{k} \in K \tag{2.1}$$

This can be viewed as evaluating a set of Fourier series coefficients due to sources with strengths c_j at the arbitrary locations $\mathbf{x}_j$. Either sign of the imaginary unit in the exponential can be chosen in the interface. Note that our normalization differs from that of references [DR,GL].

The type-2 (U to NU, aka "forward") NUFFT evaluates

$$c_j := \sum_{\mathbf{k} \in K} f_{\mathbf{k}} e^{\pm i \mathbf{k} \cdot \mathbf{x}_j} \qquad \text{for } j = 1, \dots, M \tag{2.2}$$

This is the adjoint of the type-1, ie the evaluation of a given Fourier series at a set of arbitrary points. Both type-1 and type-2 transforms are invariant under translations of the NU points by multiples of 2π, thus one could require that all NU points live in the origin-centered box $[-\pi, \pi)^d$. In fact, as a compromise between library speed, and flexibility for the user (for instance, to avoid boundary points being flagged as outside of this box due to round-off error), our library only requires that the NU points lie in the three-times-bigger box $\mathbf{x}_j \in [-3\pi, 3\pi]^d$. This allows the user to choose a convenient periodic domain that does not touch this three-times-bigger box. However, there may be a slight speed increase if most points fall in $[-\pi, \pi)^d$.

Finally, the type-3 (NU to NU) transform does not have restrictions on the NU points, and there is no periodicity. Let $\mathbf{x}_j \in \mathbb{R}^d$, $j = 1, \dots, M$, be NU locations, with strengths $c_j \in \mathbb{C}$, and let $\mathbf{s}_k$, $k = 1, \dots, N$ be NU frequencies. Then the type-3 transform evaluates:

$$f_{\mathbf{k}} := \sum_{j=1}^{M} c_j e^{\pm i \mathbf{s}_k \cdot \mathbf{x}_j} \qquad \text{for } k = 1, \dots, N \tag{2.3}$$

For all three transforms, the computational effort scales like the product of the space-bandwidth products (real-space width times frequency-space width) in each dimension. For type-1 and type-2 this means near-linear scaling in the total number of modes $N := N_1 \dots N_d$. However, be warned that for type-3 this means that, even if N and M are small, if the product of the tightest intervals enclosing the coordinates of $\mathbf{x}_j$ and $\mathbf{s}_k$ is large, the algorithm will be inefficient. For such NU points, a direct sum should be used instead.

We emphasise that the NUFFT tasks that this library performs should not be confused with either the discrete Fourier transform (DFT), the (continuous) Fourier transform (although it may be used to approximate this via a quadrature rule), or the inverse NUFFT (the iterative solution of the linear system arising from nonuniform Fourier sampling, as in, eg, MRI). It is also important to know that, for NU points, *the type-1 is not the inverse of the type-2*. See the references for clarification.

CHAPTER

THREE

CONTENTS OF THIS PACKAGE

- `finufft-manual.pdf` : the manual (auto-generated by sphinx)
- `docs` : source files for documentation (.rst files are human-readable)
- `README.md` : github-facing (and human text-reader) doc info
- `LICENSE` : how you may use this software
- `CHANGELOG` : list of changes, release notes
- `TODO` : list of things needed to fix or extend
- `makefile` : GNU makefile (there are no makefiles in subdirectories)
- `src` : main library source and headers. Compiled objects will be built here
- `lib` : dynamic library will be built here
- `lib-static` : static library will be built here
- `test` : validation and performance tests, bash scripts driving compiled C++
  - `test/check_finufft.sh` is the main pass-fail validation bash script
  - `test/nufft1testnd.sh` is a simple uniform-point performance test bash script
  - `test/results` : validation comparison outputs (*.refout; do not remove these), and local test and performance outputs (*.out; you may remove these)
- `examples` : simple example codes for calling the library from C++ and C
- `fortran` : wrappers and drivers for Fortran (see `fortran/README`)
- `matlab` : wrappers and examples for MATLAB/octave
- `finufftpy` : python wrappers
- `python_tests` : accuracy and speed tests and examples using the python wrappers
- `setup.py` : needed so pip or pip3 can build and install the python wrappers
- `contrib` : 3rd-party code

CHAPTER

FOUR

USAGE AND INTERFACES

In your C++ code you will need to include the header `src/finufft.h`. This is illustrated by the simple code `example1d1.cpp`, in the `examples` directory. From there, basic double-precision compilation with the static library is via:

```
g++ example1d1.cpp -o example1d1 ../lib-static/libfinufft.a -fopenmp -lfftw3_threads -lfftw3 -lm
```

for the default multi-threaded version, or:

```
g++ example1d1.cpp -o example1d1 ../lib-static/libfinufft.a -lfftw3 -lm
```

if you compiled FINUFFT for single-threaded only.

Interfaces from C++

You will see in `examples/example1d1.cpp` the line:

```
nufft_opts opts; finufft_default_opts(opts);
```

This is the recommended way to initialize the structure `nufft_opts` (defined in the header `../src/finufft.h`). Its fields allow control of various parameters such as the mode ordering, FFTW plan type, and text debug options (do not adjust `R`; all others are fair game). Then using the library is a matter of initializing input arrays, allocating the correct output array size, and calling one of the transform routines below.

We provide Type 1 (nonuniform to uniform), Type 2 (uniform to nonuniform), and Type 3 (nonuniform to nonuniform), in dimensions 1, 2, and 3. This gives nine routines in all.

In the below, double-precision is assumed. See next section for single-precision compilation.

1D transforms

```
int finufft1d1(BIGINT nj,double* xj,dcomplex* cj,int iflag,double eps,BIGINT ms,
               dcomplex* fk, nufft_opts opts)

Type-1 1D complex nonuniform FFT.

               nj-1
   fk(k1) =    SUM cj[j] exp(+/-i k1 xj(j))  for -ms/2 <= k1 <= (ms-1)/2
               j=0
 Inputs:
   nj     number of sources (integer of type INT; see utils.h)
   xj     nonuniform source locations, on interval [-pi,pi].
   cj     size-nj double complex array of source strengths
```

```
          (ie, stored as 2*nj doubles interleaving Re, Im).
   iflag  if >=0, uses + sign in exponential, otherwise - sign.
   eps    precision requested (>1e-16)
   ms     number of Fourier modes computed, may be even or odd;
          in either case the mode range is integers lying in [-ms/2, (ms-1)/2]
   opts   struct controlling options (see finufft.h)
 Outputs:
   fk     size-ms double complex array of Fourier transform values
          stored as alternating Re & Im parts (2*ms doubles), in
          order determined by opts.modeord.

   The type 1 NUFFT proceeds in three main steps (see [GL]):
   1) spread data to oversampled regular mesh using kernel.
   2) compute FFT on uniform mesh
   3) deconvolve by division of each Fourier mode independently by the kernel
      Fourier series coeffs (not merely FFT of kernel), shuffle to output.

 Written with FFTW style complex arrays. Step 3a internally uses dcomplex,
 and Step 3b internally uses real arithmetic and FFTW style complex.
 Because of the former, compile with -Ofast in GNU.



int finufft1d2(BIGINT nj,double* xj,dcomplex* cj,int iflag,double eps,BIGINT ms,
            dcomplex* fk, nufft_opts opts)

Type-2 1D complex nonuniform FFT.

   cj[j] = SUM   fk[k1] exp(+/-i k1 xj[j])      for j = 0,...,nj-1
           k1
   where sum is over -ms/2 <= k1 <= (ms-1)/2.

 Inputs:
   nj     number of target (integer of type INT; see utils.h)
   xj     location of targets on interval [-pi,pi].
   fk     complex Fourier transform values (size ms)
          (ie, stored as 2*nj doubles interleaving Re, Im).
   iflag  if >=0, uses + sign in exponential, otherwise - sign.
   eps    precision requested (>1e-16)
   ms     number of Fourier modes input, may be even or odd;
          in either case the mode range is integers lying in [-ms/2, (ms-1)/2]
   opts   struct controlling options (see finufft.h)
 Outputs:
   cj     complex double array of nj answers at targets

   The type 2 algorithm proceeds in three main steps (see [GL]).
   1) deconvolve (amplify) each Fourier mode, dividing by kernel Fourier coeff
   2) compute inverse FFT on uniform fine grid
   3) spread (dir=2, ie interpolate) data to regular mesh
   The kernel coeffs are precomputed in what is called step 0 in the code.

 Written with FFTW style complex arrays. Step 0 internally uses dcomplex,
 and Step 1 internally uses real arithmetic and FFTW style complex.
 Because of the former, compile with -Ofast in GNU.



int finufft1d3(BIGINT nj,double* xj,dcomplex* cj,int iflag, double eps,
```

```
               BIGINT nk, double* s, dcomplex* fk, nufft_opts opts)

Type-3 1D complex nonuniform FFT.

             nj-1
   fk[k]  =  SUM   c[j] exp(+-i s[k] xj[j]),      for k = 0, ..., nk-1
             j=0
 Inputs:
   nj     number of sources (integer of type INT; see utils.h)
   xj     location of sources in R (real line).
   cj     size-nj double complex array of source strengths
          (ie, stored as 2*nj doubles interleaving Re, Im).
   nk     number of frequency target points
   s      frequency locations of targets in R.
   iflag  if >=0, uses + sign in exponential, otherwise - sign.
   eps    precision requested (>1e-16)
   opts   struct controlling options (see finufft.h)
 Outputs:
   fk     size-nk double complex Fourier transform values at target
          frequencies sk

   The type 3 algorithm is basically a type 2 (which is implemented precisely
   as call to type 2) replacing the middle FFT (Step 2) of a type 1. See [LG].
   Beyond this, the new twists are:
   i) nf1, number of upsampled points for the type-1, depends on the product
     of interval widths containing input and output points (X*S).
   ii) The deconvolve (post-amplify) step is division by the Fourier transform
     of the scaled kernel, evaluated on the *nonuniform* output frequency
     grid; this is done by direct approximation of the Fourier integral
     using quadrature of the kernel function times exponentials.
   iii) Shifts in x (real) and s (Fourier) are done to minimize the interval
     half-widths X and S, hence nf1.

 No references to FFTW are needed here. dcomplex arithmetic is used,
 thus compile with -Ofast in GNU.
```

2D transforms

```
int finufft2d1(BIGINT nj,double* xj,double *yj,dcomplex* cj,int iflag,
               double eps, BIGINT ms, BIGINT mt, dcomplex* fk, nufft_opts opts)

Type-1 2D complex nonuniform FFT.

                   nj-1
   f[k1,k2] =      SUM  c[j] exp(+-i (k1 x[j] + k2 y[j]))
                   j=0

   for -ms/2 <= k1 <= (ms-1)/2,  -mt/2 <= k2 <= (mt-1)/2.

   The output array is k1 (fast), then k2 (slow), with each dimension
   determined by opts.modeord.
   If iflag>0 the + sign is used, otherwise the - sign is used,
   in the exponential.

 Inputs:
   nj     number of sources (integer of type INT; see utils.h)
```

```
   xj,yj     x,y locations of sources on 2D domain [-pi,pi]^2.
   cj     size-nj complex double array of source strengths,
          (ie, stored as 2*nj doubles interleaving Re, Im).
   iflag  if >=0, uses + sign in exponential, otherwise - sign.
   eps    precision requested (>1e-16)
   ms,mt  number of Fourier modes requested in x and y; each may be even or
          odd; in either case the modes are integers in [-m/2, (m-1)/2]
   opts   struct controlling options (see finufft.h)
 Outputs:
   fk     complex double array of Fourier transform values
          (size ms*mt, increasing fast in ms then slow in mt,
          ie Fortran ordering).

   The type 1 NUFFT proceeds in three main steps (see [GL]):
   1) spread data to oversampled regular mesh using kernel.
   2) compute FFT on uniform mesh
   3) deconvolve by division of each Fourier mode independently by the
      Fourier series coefficient of the kernel.
   The kernel coeffs are precomputed in what is called step 0 in the code.



int finufft2d2(BIGINT nj,double* xj,double *yj,dcomplex* cj,int iflag,double eps,
             BIGINT ms, BIGINT mt, dcomplex* fk, nufft_opts opts)

 Type-2 2D complex nonuniform FFT.

   cj[j] =  SUM   fk[k1,k2] exp(+/-i (k1 xj[j] + k2 yj[j]))      for j = 0,...,nj-1
          k1,k2
   where sum is over -ms/2 <= k1 <= (ms-1)/2, -mt/2 <= k2 <= (mt-1)/2,

 Inputs:
   nj     number of sources (integer of type INT; see utils.h)
   xj,yj     x,y locations of sources on 2D domain [-pi,pi]^2.
   fk     double complex array of Fourier transform values (size ms*mt,
          increasing fast in ms then slow in mt, ie Fortran ordering),
   iflag  if >=0, uses + sign in exponential, otherwise - sign.
   eps    precision requested (>1e-16)
   ms,mt  numbers of Fourier modes given in x and y; each may be even or odd;
          in either case the mode range is integers lying in [-m/2, (m-1)/2].
   opts   struct controlling options (see finufft.h)
 Outputs:
   cj     size-nj complex double array of source strengths

   The type 2 algorithm proceeds in three main steps (see [GL]).
   1) deconvolve (amplify) each Fourier mode, dividing by kernel Fourier coeff
   2) compute inverse FFT on uniform fine grid
   3) spread (dir=2, ie interpolate) data to regular mesh
   The kernel coeffs are precomputed in what is called step 0 in the code.



int finufft2d3(BIGINT nj,double* xj,double* yj,dcomplex* cj,int iflag,
    double eps, BIGINT nk, double* s, double *t, dcomplex* fk, nufft_opts opts)

 Type-3 2D complex nonuniform FFT.

             nj-1
```

```
   fk[k]  =  SUM   c[j] exp(+-i (s[k] xj[j] + t[k] yj[j]),    for k=0,...,nk-1
             j=0
 Inputs:
   nj     number of sources (integer of type INT; see utils.h)
   xj,yj  x,y location of sources in R^2.
   cj     size-nj complex double array of source strengths,
          (ie, stored as 2*nj doubles interleaving Re, Im).
   nk     number of frequency target points
   s,t    (k_x,k_y) frequency locations of targets in R^2.
   iflag  if >=0, uses + sign in exponential, otherwise - sign.
   eps    precision requested (>1e-16)
   opts   struct controlling options (see finufft.h)
 Outputs:
   fk     complex double Fourier transform values at the target frequencies sk

   The type 3 algorithm is basically a type 2 (which is implemented precisely
   as call to type 2) replacing the middle FFT (Step 2) of a type 1. See [LG].
   Beyond this, the new twists are:
   i) number of upsampled points for the type-1 in each dim, depends on the
     product of interval widths containing input and output points (X*S), for
     that dim.
   ii) The deconvolve (post-amplify) step is division by the Fourier transform
     of the scaled kernel, evaluated on the *nonuniform* output frequency
     grid; this is done by direct approximation of the Fourier integral
     using quadrature of the kernel function times exponentials.
   iii) Shifts in x (real) and s (Fourier) are done to minimize the interval
     half-widths X and S, hence nf, in each dim.

 No references to FFTW are needed here. Some dcomplex arithmetic is used,
 thus compile with -Ofast in GNU.
```

3D transforms

```
int finufft3d1(BIGINT nj,double* xj,double *yj,double *zj,dcomplex* cj,int iflag,
               double eps, BIGINT ms, BIGINT mt, BIGINT mu, dcomplex* fk,
               nufft_opts opts)

 Type-1 3D complex nonuniform FFT.

                     nj-1
   f[k1,k2,k3] =     SUM  c[j] exp(+-i (k1 x[j] + k2 y[j] + k3 z[j]))
                     j=0

      for -ms/2 <= k1 <= (ms-1)/2,  -mt/2 <= k2 <= (mt-1)/2,
          -mu/2 <= k3 <= (mu-1)/2.

   In the output array, k1 is fastest, k2 middle, and k3 slowest, ie
   Fortran ordering, with each dimension
   determined by opts.modeord. If iflag>0 the + sign is used, otherwise the -
   sign is used, in the exponential.

 Inputs:
   nj     number of sources (integer of type INT; see utils.h)
   xj,yj,zj   x,y,z locations of sources on 3D domain [-pi,pi]^3.
   cj     size-nj complex double array of source strengths,
          (ie, stored as 2*nj doubles interleaving Re, Im).
```

```
   iflag  if >=0, uses + sign in exponential, otherwise - sign.
   eps    precision requested
   ms,mt,mu  number of Fourier modes requested in x,y,z;
          each may be even or odd;
          in either case the mode range is integers lying in [-m/2, (m-1)/2]
   opts   struct controlling options (see finufft.h)
 Outputs:
   fk     complex double array of Fourier transform values (size ms*mt*mu,
          increasing fast in ms to slowest in mu, ie Fortran ordering).

   The type 1 NUFFT proceeds in three main steps (see [GL]):
   1) spread data to oversampled regular mesh using kernel.
   2) compute FFT on uniform mesh
   3) deconvolve by division of each Fourier mode independently by the
      Fourier series coefficient of the kernel.
   The kernel coeffs are precomputed in what is called step 0 in the code.



int finufft3d2(BIGINT nj,double* xj,double *yj,double *zj,dcomplex* cj,
               int iflag,double eps, BIGINT ms, BIGINT mt, BIGINT mu,
               dcomplex* fk, nufft_opts opts)

 Type-2 3D complex nonuniform FFT.

   cj[j] =    SUM   fk[k1,k2,k3] exp(+/-i (k1 xj[j] + k2 yj[j] + k3 zj[j]))
            k1,k2,k3
    for j = 0,...,nj-1
   where sum is over -ms/2 <= k1 <= (ms-1)/2, -mt/2 <= k2 <= (mt-1)/2,
                     -mu/2 <= k3 <= (mu-1)/2

 Inputs:
   nj     number of sources (integer of type INT; see utils.h)
   xj,yj,zj     x,y,z locations of sources on 3D domain [-pi,pi]^3.
   fk     double complex array of Fourier series values (size ms*mt*mu,
          fastest in ms to slowest in mu, ie Fortran ordering).
          (ie, stored as alternating Re & Im parts, 2*ms*mt*mu doubles)
   iflag  if >=0, uses + sign in exponential, otherwise - sign.
   eps    precision requested
   ms,mt,mu  numbers of Fourier modes given in x,y,z; each may be even or odd;
          in either case the mode range is integers lying in [-m/2, (m-1)/2].
   opts   struct controlling options (see finufft.h)
 Outputs:
   cj     size-nj complex double array of target values,
          (ie, stored as 2*nj doubles interleaving Re, Im).

   The type 2 algorithm proceeds in three main steps (see [GL]).
   1) deconvolve (amplify) each Fourier mode, dividing by kernel Fourier coeff
   2) compute inverse FFT on uniform fine grid
   3) spread (dir=2, ie interpolate) data to regular mesh
   The kernel coeffs are precomputed in what is called step 0 in the code.



int finufft3d3(BIGINT nj,double* xj,double* yj,double *zj, dcomplex* cj,
               int iflag, double eps, BIGINT nk, double* s, double *t,
               double *u, dcomplex* fk, nufft_opts opts)
```

```
Type-3 3D complex nonuniform FFT.

             nj-1
  fk[k]  =   SUM   c[j] exp(+-i (s[k] xj[j] + t[k] yj[j] + u[k] zj[j]),
             j=0
                        for k=0,...,nk-1
Inputs:
  nj     number of sources (integer of type INT; see utils.h)
  xj,yj,zj   x,y,z location of sources in R^3.
  cj     size-nj complex double array of source strengths
         (ie, interleaving Re & Im parts)
  nk     number of frequency target points
  s,t,u      (k_x,k_y,k_z) frequency locations of targets in R^3.
  iflag  if >=0, uses + sign in exponential, otherwise - sign.
  eps    precision requested
  opts   struct controlling options (see finufft.h)
Outputs:
  fk     size-nk complex double array of Fourier transform values at the
         target frequencies sk

  The type 3 algorithm is basically a type 2 (which is implemented precisely
  as call to type 2) replacing the middle FFT (Step 2) of a type 1. See [LG].
  Beyond this, the new twists are:
  i) number of upsampled points for the type-1 in each dim, depends on the
    product of interval widths containing input and output points (X*S), for
    that dim.
  ii) The deconvolve (post-amplify) step is division by the Fourier transform
    of the scaled kernel, evaluated on the *nonuniform* output frequency
    grid; this is done by direct approximation of the Fourier integral
    using quadrature of the kernel function times exponentials.
  iii) Shifts in x (real) and s (Fourier) are done to minimize the interval
    half-widths X and S, hence nf, in each dim.

No references to FFTW are needed here. Some dcomplex arithmetic is used,
thus compile with -Ofast in GNU.
```

Custom library compilation options

You may want to make the library for other data types. Currently this overwrites the same library names, so you will have to move them to other locations if you want to keep both versions for use together.

1. Use `make [task] PREC=SINGLE` for single-precision, otherwise will be double-precision. Single-precision saves half the RAM, and increases speed slightly (<20%). The C++, C, and fortran demos are all tested in single precision. However, it will break matlab, octave, python interfaces.
2. make with OMP=OFF for single-threaded, otherwise multi-threaded (openmp).
3. If you want to restrict to array sizes <2^31 and explore if 32-bit integer indexing beats 64-bit, add flag `-DSMALLINT` to `CXXFLAGS` which sets `BIGINT` to `int`.
4. If you want 32 bit integers in the FINUFFT library interface instead of `int64`, add flag `-DINTERFACE32` (experimental; C,F,M,O interfaces will break)

More information about large arrays:

By default FINUFFT uses 64-bit integers internally and for interfacing; this means arguments such as the number of sources (`nj`) are type int64_t, allowing `nj` to equal or exceed 2^31 (around 2e9).

There is a chance the user may want to compile a custom version with 32-bit integers internally (although we have not noticed a speed increase on a modern CPU). In the makefile one may add the compile flag `-DSMALLINT` for this, which changes `BIGINT` from `int64_t` to `int`.

Similarly, the user may want to change the integer interface type to 32-bit ints. The compile flag `-DINTERFACE32` does this, and changes `INT` from `int64_t` to `int`.

See `../src/utils.h` for these typedefs.

Sizes >=2^31 have been tested for C++ drivers (`test/finufft?d_test.cpp`), and work fine, if you have enough RAM.

In fortran and C the interface is still 32-bit integers, limiting to array sizes <2^31.

In Matlab/MEX, mwrap uses `int` types, so that output arrays can *only* be <2^31. However, input arrays >=2^31 have been tested, and while they don't crash, they result in wrong answers (all zeros). This is yet to be fixed.

Design notes and advanced usage

C++ is used for all main libraries, almost entirely avoiding object-oriented code. C++ `std::complex<double>` (aliased to `dcomplex`) and FFTW complex types are mixed within the library, since to some extent it is a glorified driver for FFTW. The interfaces are dcomplex. FFTW was considered universal and essential enough to be a dependency for the whole package.

The default FFTW plan is `FFTW_ESTIMATE`; however if you will be making multiple calls, consider using `opts` to set `fftw=FFTW_MEASURE`, which will spend many seconds planning but give the fastest speed when called again. Note that FFTW plans are saved automatically from call to call in the same executable, and the same MATLAB session.

There is a hard-defined limit of `1e11` for internal FFT arrays, set in `common.h`; if your machine has RAM of order 1TB, and you need it, set this larger and recompile. The point of this is to catch ridiculous-sized mallocs and exit gracefully. Note that mallocs smaller than this, but which still exceed available RAM, cause segfaults as usual. For simplicity of code, we do not do error checking on every malloc.

As a spreading kernel function, we use a new faster simplification of the Kaiser–Bessel kernel. At high requested precisions, like the Kaiser–Bessel, this achieves roughly half the kernel width achievable by a truncated Gaussian. Our kernel is exp(-beta.sqrt(1-(2x/W)^2)), where W = nspread is the full kernel width in grid units. This (and Kaiser–Bessel) are good approximations to the prolate spheroidal wavefunction of order zero (PSWF), being the functions of given support [-W/2,W/2] whose Fourier transform has minimal L2 norm outside a symmetric interval. The PSWF frequency parameter (see [ORZ]) is c = pi.(1-1/2R).W where R is the upsampling parameter (currently R=2.0).

Known issues and bug reports

- When requestes accuracy is `1e-14` or less, it is sometimes not possible to match this, especially when there are a large number of input and/or output points. This is believed to be unavoidable round-off error.
- Currently in Mac OSX, `make lib` fails to make the shared object library (.so).
- The timing of FFTW calls is complicated, depending on whether FFTW_ESTIMATE (the default) or FFTW_MEASURE is used. Such issues are known, and discussed in other documentation, eg https://pythonhosted.org/poppy/fft_optimization.html
- MATLAB, octave and python cannot exceed input or output data sizes of 2^31.

Also see notes in the `TODO` file.

If you think you have found a bug, please contact Alex Barnett (`abarnett` at-sign `flatironinstitute.org`) with FINUFFT in the subject line. Include a minimal code which reproduces the bug, along with details about your machine, operating system, compiler, and version of FINUFFT.

CHAPTER

FIVE

MATLAB/OCTAVE INTERFACES

```
---------------------------------------------------------------------
FINUFFT1D1

[f ier] = finufft1d1(x,c,isign,eps,ms)
[f ier] = finufft1d1(x,c,isign,eps,ms,opts)

Type-1 1D complex nonuniform FFT.

               nj
    f(k1) =  SUM c[j] exp(+/-i k1 x(j))  for -ms/2 <= k1 <= (ms-1)/2
             j=1
  Inputs:
    x     location of sources on interval [-3pi,3pi], length nj
    c     size-nj complex array of source strengths
    isign  if >=0, uses + sign in exponential, otherwise - sign.
    eps     precision requested (>1e-16)
    ms     number of Fourier modes computed, may be even or odd;
           in either case the mode range is integers lying in [-ms/2, (ms-1)/2]
    opts.debug: 0 (silent, default), 1 (timing breakdown), 2 (debug info).
    opts.nthreads sets requested number of threads (else automatic)
    opts.spread_sort: 0 (don't sort NU pts in spreader), 1 (sort, default)
    opts.fftw: 0 (use FFTW_ESTIMATE, default), 1 (use FFTW_MEASURE)
    opts.modeord: 0 (CMCL increasing mode ordering, default), 1 (FFT ordering)
    opts.chkbnds: 0 (don't check NU points valid), 1 (do, default).
  Outputs:
    f     size-ms double complex array of Fourier transform values
    ier - 0 if success, else:
                    1 : eps too small
                     2 : size of arrays to malloc exceed MAX_NF
                    other codes: as returned by cnufftspread
---------------------------------------------------------------------------
FINUFFT1D2

[c ier] = finufft1d2(x,isign,eps,f)
[c ier] = finufft1d2(x,isign,eps,f,opts)

Type-2 1D complex nonuniform FFT.

   c[j] = SUM   f[k1] exp(+/-i k1 x[j])      for j = 1,...,nj
           k1
    where sum is over -ms/2 <= k1 <= (ms-1)/2.

 Inputs:
    x     location of NU targets on interval [-3pi,3pi], length nj
    f     complex Fourier transform values
```

```
    isign  if >=0, uses + sign in exponential, otherwise - sign.
    eps    precision requested (>1e-16)
    opts.debug: 0 (silent, default), 1 (timing breakdown), 2 (debug info).
    opts.nthreads sets requested number of threads (else automatic)
    opts.spread_sort: 0 (don't sort NU pts in spreader), 1 (sort, default)
    opts.fftw: 0 (use FFTW_ESTIMATE, default), 1 (use FFTW_MEASURE)
    opts.modeord: 0 (CMCL increasing mode ordering, default), 1 (FFT ordering)
    opts.chkbnds: 0 (don't check NU points valid), 1 (do, default).
 Outputs:
    c     complex double array of nj answers at targets
    ier - 0 if success, else:
                   1 : eps too small
                           2 : size of arrays to malloc exceed MAX_NF
                   other codes: as returned by cnufftspread
c = complex(zeros(nj,1));   % todo: change all output to inout & prealloc...
------------------------------------------------------------------------
FINUFFT1D3

[f ier] = finufft1d3(x,c,isign,eps,s)
[f ier] = finufft1d3(x,c,isign,eps,s,opts)

             nj
    f[k]  =  SUM   c[j] exp(+-i s[k] x[j]),      for k = 1, ..., nk
             j=1
  Inputs:
    x      location of NU sources in R (real line).
    c      size-nj double complex array of source strengths
    s      frequency locations of NU targets in R.
    isign  if >=0, uses + sign in exponential, otherwise - sign.
    eps    precision requested (>1e-16)
    opts.debug: 0 (silent, default), 1 (timing breakdown), 2 (debug info).
    opts.nthreads sets requested number of threads (else automatic)
    opts.spread_sort: 0 (don't sort NU pts in spreader), 1 (sort, default)
    opts.fftw: 0 (use FFTW_ESTIMATE, default), 1 (use FFTW_MEASURE)
  Outputs:
    f     size-nk double complex Fourier transform values at target
           frequencies s
    returned value - 0 if success, else:
                     1 : eps too small
                      2 : size of arrays to malloc exceed MAX_NF
------------------------------------------------------------------------
FINUFFT2D1

[f ier] = finufft2d1(x,y,c,isign,eps,ms,mt)
[f ier] = finufft2d1(x,y,c,isign,eps,ms,mt,opts)

Type-1 2D complex nonuniform FFT.

                  nj
    f[k1,k2] =   SUM  c[j] exp(+-i (k1 x[j] + k2 y[j]))
                 j=1

    for -ms/2 <= k1 <= (ms-1)/2,  -mt/2 <= k2 <= (mt-1)/2.

  Inputs:
    x,y   locations of NU sources on the square [-3pi,3pi]^2, each length nj
    c     size-nj complex array of source strengths
    isign  if >=0, uses + sign in exponential, otherwise - sign.
```

```
    eps     precision requested (>1e-16)
    ms,mt  number of Fourier modes requested in x & y; each may be even or odd
          in either case the mode range is integers lying in [-m/2, (m-1)/2]
    opts.debug: 0 (silent, default), 1 (timing breakdown), 2 (debug info).
    opts.nthreads sets requested number of threads (else automatic)
    opts.spread_sort: 0 (don't sort NU pts in spreader), 1 (sort, default)
    opts.fftw: 0 (use FFTW_ESTIMATE, default), 1 (use FFTW_MEASURE)
    opts.modeord: 0 (CMCL increasing mode ordering, default), 1 (FFT ordering)
    opts.chkbnds: 0 (don't check NU points valid), 1 (do, default).
  Outputs:
    f     size (ms*mt) double complex array of Fourier transform values
          (ordering given by opts.modeord in each dimension, ms fast, mt slow)
    ier - 0 if success, else:
                    1 : eps too small
                     2 : size of arrays to malloc exceed MAX_NF
                    other codes: as returned by cnufftspread
-------------------------------------------------------------------------
FINUFFT2D2

[c ier] = finufft2d2(x,y,isign,eps,f)
[c ier] = finufft2d2(x,y,isign,eps,f,opts)

Type-2 2D complex nonuniform FFT.

   c[j] =  SUM   f[k1,k2] exp(+/-i (k1 x[j] + k2 y[j]))  for j = 1,..,nj
          k1,k2
    where sum is over -ms/2 <= k1 <= (ms-1)/2, -mt/2 <= k2 <= (mt-1)/2,

 Inputs:
    x,y   location of NU targets on the square [-3pi,3pi]^2, each length nj
    f     size (ms,mt) complex Fourier transform value matrix
          (mode ordering given by opts.modeord in each dimension)
    isign  if >=0, uses + sign in exponential, otherwise - sign.
    eps    precision requested (>1e-16)
    opts.debug: 0 (silent, default), 1 (timing breakdown), 2 (debug info).
    opts.nthreads sets requested number of threads (else automatic)
    opts.spread_sort: 0 (don't sort NU pts in spreader), 1 (sort, default)
    opts.fftw: 0 (use FFTW_ESTIMATE, default), 1 (use FFTW_MEASURE)
    opts.modeord: 0 (CMCL increasing mode ordering, default), 1 (FFT ordering)
    opts.chkbnds: 0 (don't check NU points valid), 1 (do, default).
 Outputs:
    c     complex double array of nj answers at the targets.
    ier - 0 if success, else:
                    1 : eps too small
                           2 : size of arrays to malloc exceed MAX_NF
                    other codes: as returned by cnufftspread
-------------------------------------------------------------------------
FINUFFT2D3

[f ier] = finufft2d3(x,y,c,isign,eps,s,t)
[f ier] = finufft2d3(x,y,c,isign,eps,s,t,opts)

             nj
    f[k]  =  SUM   c[j] exp(+-i (s[k] x[j] + t[k] y[j])),  for k = 1, ..., nk
             j=1
  Inputs:
    x,y    location of NU sources in R^2, each length nj.
    c      size-nj double complex array of source strengths
```

```
    s,t    frequency locations of NU targets in R^2.
    isign  if >=0, uses + sign in exponential, otherwise - sign.
    eps    precision requested (>1e-16)
    opts.debug: 0 (silent, default), 1 (timing breakdown), 2 (debug info).
    opts.nthreads sets requested number of threads (else automatic)
    opts.spread_sort: 0 (don't sort NU pts in spreader), 1 (sort, default)
    opts.fftw: 0 (use FFTW_ESTIMATE, default), 1 (use FFTW_MEASURE)
  Outputs:
    f     size-nk double complex Fourier transform values at target
           frequencies s,t
    returned value - 0 if success, else:
                     1 : eps too small
                      2 : size of arrays to malloc exceed MAX_NF
-------------------------------------------------------------------------
FINUFFT3D1

[f ier] = finufft3d1(x,y,z,c,isign,eps,ms,mt,mu)
[f ier] = finufft3d1(x,y,z,c,isign,eps,ms,mt,mu,opts)

Type-1 3D complex nonuniform FFT.

                       nj
    f[k1,k2,k3] =     SUM  c[j] exp(+-i (k1 x[j] + k2 y[j] + k3 z[j]))
                      j=1

    for -ms/2 <= k1 <= (ms-1)/2,  -mt/2 <= k2 <= (mt-1)/2,
        -mu/2 <= k3 <= (mu-1)/2.

  Inputs:
    x,y,z locations of NU sources on [-3pi,3pi]^3, each length nj
    c     size-nj complex array of source strengths
    isign  if >=0, uses + sign in exponential, otherwise - sign.
    eps     precision requested (>1e-16)
    ms,mt,mu number of Fourier modes requested in x,y and z; each may be
          even or odd.
          In either case the mode range is integers lying in [-m/2, (m-1)/2]
    opts.debug: 0 (silent, default), 1 (timing breakdown), 2 (debug info).
    opts.nthreads sets requested number of threads (else automatic)
    opts.spread_sort: 0 (don't sort NU pts in spreader), 1 (sort, default)
    opts.fftw: 0 (use FFTW_ESTIMATE, default), 1 (use FFTW_MEASURE)
    opts.modeord: 0 (CMCL increasing mode ordering, default), 1 (FFT ordering)
    opts.chkbnds: 0 (don't check NU points valid), 1 (do, default).
  Outputs:
    f     size (ms*mt*mu) double complex array of Fourier transform values
           (ordering given by opts.modeord in each dimension, ms fastest, mu
            slowest).
    ier - 0 if success, else:
                    1 : eps too small
                     2 : size of arrays to malloc exceed MAX_NF
                    other codes: as returned by cnufftspread
-------------------------------------------------------------------------
FINUFFT3D2

[c ier] = finufft3d2(x,y,z,isign,eps,f)
[c ier] = finufft3d2(x,y,z,isign,eps,f,opts)

Type-2 3D complex nonuniform FFT.
```

```
   c[j] =   SUM   f[k1,k2,k3] exp(+/-i (k1 x[j] + k2 y[j] + k3 z[j]))
          k1,k2,k3
                           for j = 1,..,nj
    where sum is over -ms/2 <= k1 <= (ms-1)/2, -mt/2 <= k2 <= (mt-1)/2,
                      -mu/2 <= k3 <= (mu-1)/2.

 Inputs:
    x,y,z location of NU targets on cube [-3pi,3pi]^3, each length nj
    f     size (ms,mt,mu) complex Fourier transform value matrix
          (ordering given by opts.modeord in each dimension; ms fastest to mu
           slowest).
    isign  if >=0, uses + sign in exponential, otherwise - sign.
    eps    precision requested (>1e-16)
    opts.debug: 0 (silent, default), 1 (timing breakdown), 2 (debug info).
    opts.nthreads sets requested number of threads (else automatic)
    opts.spread_sort: 0 (don't sort NU pts in spreader), 1 (sort, default)
    opts.fftw: 0 (use FFTW_ESTIMATE, default), 1 (use FFTW_MEASURE)
    opts.modeord: 0 (CMCL increasing mode ordering, default), 1 (FFT ordering)
    opts.chkbnds: 0 (don't check NU points valid), 1 (do, default).
 Outputs:
    c     complex double array of nj answers at the targets.
    ier - 0 if success, else:
                    1 : eps too small
                           2 : size of arrays to malloc exceed MAX_NF
                    other codes: as returned by cnufftspread
------------------------------------------------------------------------------
FINUFFT3D3

[f ier] = finufft3d3(x,y,z,c,isign,eps,s,t,u)
[f ier] = finufft3d3(x,y,z,c,isign,eps,s,t,u,opts)

             nj
    f[k]  =  SUM   c[j] exp(+-i (s[k] x[j] + t[k] y[j] + u[k] z[j])),
             j=1
                            for k = 1, ..., nk
  Inputs:
    x,y,z  location of NU sources in R^3, each length nj.
    c      size-nj double complex array of source strengths
    s,t,u   frequency locations of NU targets in R^3.
    isign  if >=0, uses + sign in exponential, otherwise - sign.
    eps    precision requested (>1e-16)
    opts.debug: 0 (silent, default), 1 (timing breakdown), 2 (debug info).
    opts.nthreads sets requested number of threads (else automatic)
    opts.spread_sort: 0 (don't sort NU pts in spreader), 1 (sort, default)
    opts.fftw: 0 (use FFTW_ESTIMATE, default), 1 (use FFTW_MEASURE)
  Outputs:
    f     size-nk double complex Fourier transform values at target
           frequencies s,t,u
    returned value - 0 if success, else:
                     1 : eps too small
                      2 : size of arrays to malloc exceed MAX_NF
------------------------------------------------------------------------
```

CHAPTER

SIX

PYTHON INTERFACES TO FINUFFT

These python interfaces are by Daniel Foreman-Mackey, Jeremy Magland, and Alex Barnett, with help from David Stein. See the installation notes for how to install these interfaces. Below is the documentation for the nine routines.

Notes:

1. The module has been designed not to recompile the C++ library; rather, it links to the existing static library.
2. In the below, "float" and "complex" refer to double-precision for the default library. One can compile the library for single-precision, but the python interfaces are untested in this case.
3. NumPy input and output arrays are generally passed directly without copying, which helps efficiency in large low-accuracy problems. In 2D and 3D, copying is avoided when arrays are Fortran-ordered; hence choose this ordering in your python code if you are able (see `python_tests/accuracy_speed_tests.py`).
4. Fortran-style writing of the output to a preallocated NumPy input array is used. That is, such an array is treated as a pointer into which the output is written. This avoids creation of new arrays. The python call return value is merely a status indicator.

`finufftpy.`**`nufft1d1`**(*x*, *c*, *isign*, *eps*, *ms*, *f*, *debug=0*, *spread_debug=0*, *spread_sort=1*, *fftw=0*, *modeord=0*, *chkbnds=1*)

1D type-1 (aka adjoint) complex nonuniform fast Fourier transform

```
             nj-1
f(k1) =      SUM c[j] exp(+/-i k1 x(j))   for -ms/2 <= k1 <= (ms-1)/2
             j=0
```

Parameters

- **`x`** (*`float[nj]`*) – nonuniform source points, valid only in [-3pi,3pi]
- **`c`** (*`complex[nj]`*) – source strengths
- **`isign`** (*`int`*) – if >=0, uses + sign in exponential, otherwise - sign
- **`eps`** (*`float`*) – precision requested (>1e-16)
- **`ms`** (*`int`*) – number of Fourier modes requested, may be even or odd; in either case the modes are integers lying in [-ms/2, (ms-1)/2]
- **`f`** (*`complex[ms]`*) – output Fourier mode values. Should be initialized as a numpy array of the correct size
- **`debug`** (*`int, optional`*) – 0 (silent), 1 (print timing breakdown).
- **`spread_debug`** (*`int, optional`*) – 0 (silent), 1, 2... (prints spreader info)
- **`spread_sort`** (*`int, optional`*) – 0 (don't sort NU pts in spreader), 1 (sort)
- **`fftw`** (*`int, optional`*) – 0 (use FFTW_ESTIMATE), 1 (use FFTW_MEASURE)

- **modeord** (*int, optional*) – 0 (CMCL increasing mode ordering), 1 (FFT ordering)
- **chkbnds** (*int, optional*) – 0 (don't check NU points valid), 1 (do)

Note: The output is written into the f array.

Returns 0 if success, 1 if eps too small, 2 if size of arrays to malloc exceed MAX_NF, 4 at least one NU point out of range (if chkbnds true)

Return type int

Example

see `python_tests/demo1d1.py`

`finufftpy.`**nufft1d2**(*x*, *c*, *isign*, *eps*, *f*, *debug=0*, *spread_debug=0*, *spread_sort=1*, *fftw=0*, *modeord=0*, *chkbnds=1*)

1D type-2 (aka forward) complex nonuniform fast Fourier transform

```
    c[j] = SUM   f[k1] exp(+/-i k1 x[j])      for j = 0,...,nj-1
            k1

        where sum is over -ms/2 <= k1 <= (ms-1)/2.
```

Parameters

- **x** (*float[nj]*) – nonuniform target points, valid only in [-3pi,3pi]
- **c** (*complex[nj]*) – output values at targets. Should be initialized as a numpy array of the correct size
- **isign** (*int*) – if >=0, uses + sign in exponential, otherwise - sign
- **eps** (*float*) – precision requested (>1e-16)
- **f** (*complex[ms]*) – Fourier mode coefficients, where ms is even or odd In either case the mode indices are integers in [-ms/2, (ms-1)/2]
- **debug** (*int, optional*) – 0 (silent), 1 (print timing breakdown)
- **spread_debug** (*int, optional*) – 0 (silent), 1, 2... (print spreader info)
- **spread_sort** (*int, optional*) – 0 (don't sort NU pts in spreader), 1 (sort)
- **fftw** (*int, optional*) – 0 (use FFTW_ESTIMATE), 1 (use FFTW_MEASURE)
- **modeord** (*int, optional*) – 0 (CMCL increasing mode ordering), 1 (FFT ordering)
- **chkbnds** (*int, optional*) – 0 (don't check NU points valid), 1 (do)

Note: The output is written into the c array.

Returns 0 if success, 1 if eps too small, 2 if size of arrays to malloc exceed MAX_NF, 4 at least one NU point out of range (if chkbnds true)

Return type int

Example

see `python_tests/accuracy_speed_tests.py`

`finufftpy.`**`nufft1d3`**(*x*, *c*, *isign*, *eps*, *s*, *f*, *debug=0*, *spread_debug=0*, *spread_sort=1*, *fftw=0*)

1D type-3 (NU-to-NU) complex nonuniform fast Fourier transform

```
             nj-1
    f[k]  =  SUM   c[j] exp(+-i s[k] x[j]),      for k = 0, ..., nk-1
             j=0
```

Parameters

- **x** (*float[nj]*) – nonuniform source points, in R
- **c** (*complex[nj]*) – source strengths
- **isign** (*int*) – if >=0, uses + sign in exponential, otherwise - sign
- **eps** (*float*) – precision requested (>1e-16)
- **s** (*float[nk]*) – nonuniform target frequency points, in R
- **f** (*complex[nk]*) – output values at target frequencies. Should be initialized as a numpy array of the correct size
- **debug** (*int, optional*) – 0 (silent), 1 (print timing breakdown)
- **spread_debug** (*int, optional*) – 0 (silent), 1, 2... (print spreader info)
- **spread_sort** (*int, optional*) – 0 (don't sort NU pts in spreader), 1 (sort)
- **fftw** (*int, optional*) – 0 (use FFTW_ESTIMATE), 1 (use FFTW_MEASURE)

Note: The output is written into the f array.

Returns 0 if success, 1 if eps too small, 2 if size of arrays to malloc exceed MAX_NF

Return type int

Example

see `python_tests/accuracy_speed_tests.py`

`finufftpy.`**`nufft2d1`**(*x*, *y*, *c*, *isign*, *eps*, *ms*, *mt*, *f*, *debug=0*, *spread_debug=0*, *spread_sort=1*, *fftw=0*, *modeord=0*, *chkbnds=1*)

2D type-1 (aka adjoint) complex nonuniform fast Fourier transform

```
                nj-1
    f(k1,k2) =  SUM c[j] exp(+/-i (k1 x(j) + k2 y[j])),
                j=0
                      for -ms/2 <= k1 <= (ms-1)/2, -mt/2 <= k2 <= (mt-1)/2
```

Parameters

- **x** (*float[nj]*) – nonuniform source x-coords, valid only in [-3pi,3pi]
- **y** (*float[nj]*) – nonuniform source y-coords, valid only in [-3pi,3pi]
- **c** (*complex[nj]*) – source strengths

- **isign** (*int*) – if >=0, uses + sign in exponential, otherwise - sign
- **eps** (*float*) – precision requested (>1e-16)
- **ms** (*int*) – number of Fourier modes in x-direction, may be even or odd; in either case the modes are integers lying in [-ms/2, (ms-1)/2]
- **mt** (*int*) – number of Fourier modes in y-direction, may be even or odd; in either case the modes are integers lying in [-mt/2, (mt-1)/2]
- **f** (*complex[ms,mt]*) – output Fourier mode values. Should be initialized as a Fortran-ordered (ie ms fast, mt slow) numpy array of the correct size
- **debug** (*int, optional*) – 0 (silent), 1 (print timing breakdown)
- **spread_debug** (*int, optional*) – 0 (silent), 1, 2... (prints spreader info)
- **spread_sort** (*int, optional*) – 0 (don't sort NU pts in spreader), 1 (sort)
- **fftw** (*int, optional*) – 0 (use FFTW_ESTIMATE), 1 (use FFTW_MEASURE)
- **modeord** (*int, optional*) – 0 (CMCL increasing mode ordering), 1 (FFT ordering)
- **chkbnds** (*int, optional*) – 0 (don't check NU points valid), 1 (do)

Note: The output is written into the f array.

Returns 0 if success, 1 if eps too small, 2 if size of arrays to malloc exceed MAX_NF, 4 at least one NU point out of range (if chkbnds true)

Return type int

Example

see `python/tests/accuracy_speed_tests.py`

`finufftpy.`**`nufft2d2`**(*x*, *y*, *c*, *isign*, *eps*, *f*, *debug=0*, *spread_debug=0*, *spread_sort=1*, *fftw=0*, *modeord=0*, *chkbnds=1*)

2D type-2 (aka forward) complex nonuniform fast Fourier transform

```
    c[j] =   SUM   f[k1,k2] exp(+/-i (k1 x[j] + k2 y[j])),  for j = 0,...,nj-1
            k1,k2

    where sum is over -ms/2 <= k1 <= (ms-1)/2, -mt/2 <= k2 <= (mt-1)/2
```

Parameters

- **x** (*float[nj]*) – nonuniform target x-coords, valid only in [-3pi,3pi]
- **y** (*float[nj]*) – nonuniform target y-coords, valid only in [-3pi,3pi]
- **c** (*complex[nj]*) – output values at targets. Should be initialized as a numpy array of the correct size
- **isign** (*int*) – if >=0, uses + sign in exponential, otherwise - sign
- **eps** (*float*) – precision requested (>1e-16)
- **f** (*complex[ms,mt]*) – Fourier mode coefficients, where ms and mt are either even or odd; in either case their mode range is integers lying in [-m/2, (m-1)/2], with mode ordering in all dimensions given by modeord. Ordering is Fortran-style, ie ms fastest.

- **debug** (*int, optional*) – 0 (silent), 1 (print timing breakdown)
- **spread_debug** (*int, optional*) – 0 (silent), 1, 2... (print spreader info)
- **spread_sort** (*int, optional*) – 0 (don't sort NU pts in spreader), 1 (sort)
- **fftw** (*int, optional*) – 0 (use FFTW_ESTIMATE), 1 (use FFTW_MEASURE)
- **modeord** (*int, optional*) – 0 (CMCL increasing mode ordering), 1 (FFT ordering)
- **chkbnds** (*int, optional*) – 0 (don't check NU points valid), 1 (do)

Note: The output is written into the c array.

Returns 0 if success, 1 if eps too small, 2 if size of arrays to malloc exceed MAX_NF, 4 at least one NU point out of range (if chkbnds true)

Return type int

Example

see `python_tests/accuracy_speed_tests.py`

`finufftpy.`**`nufft2d3`**(*x*, *y*, *c*, *isign*, *eps*, *s*, *t*, *f*, *debug=0*, *spread_debug=0*, *spread_sort=1*, *fftw=0*)

2D type-3 (NU-to-NU) complex nonuniform fast Fourier transform

```
             nj-1
f[k]   =     SUM   c[j] exp(+-i s[k] x[j] + t[k] y[j]),  for k = 0,...,nk-1
             j=0
```

Parameters

- **x** (*float[nj]*) – nonuniform source point x-coords, in R
- **y** (*float[nj]*) – nonuniform source point y-coords, in R
- **c** (*complex[nj]*) – source strengths
- **isign** (*int*) – if >=0, uses + sign in exponential, otherwise - sign
- **eps** (*float*) – precision requested (>1e-16)
- **s** (*float[nk]*) – nonuniform target x-frequencies, in R
- **t** (*float[nk]*) – nonuniform target y-frequencies, in R
- **f** (*complex[nk]*) – output values at target frequencies. Should be initialized as a numpy array of the correct size
- **debug** (*int, optional*) – 0 (silent), 1 (print timing breakdown)
- **spread_debug** (*int, optional*) – 0 (silent), 1, 2... (print spreader info)
- **spread_sort** (*int, optional*) – 0 (don't sort NU pts in spreader), 1 (sort)
- **fftw** (*int, optional*) – 0 (use FFTW_ESTIMATE), 1 (use FFTW_MEASURE)

Note: The output is written into the f array.

Returns 0 if success, 1 if eps too small, 2 if size of arrays to malloc exceed MAX_NF

Return type int

Example

see `python_tests/accuracy_speed_tests.py`

`finufftpy.`**`nufft3d1`**(*x*, *y*, *z*, *c*, *isign*, *eps*, *ms*, *mt*, *mu*, *f*, *debug=0*, *spread_debug=0*, *spread_sort=1*, *fftw=0*, *modeord=0*, *chkbnds=1*)

3D type-1 (aka adjoint) complex nonuniform fast Fourier transform

```
                    nj-1
    f(k1,k2,k3) =   SUM c[j] exp(+/-i (k1 x(j) + k2 y[j] + k3 z[j])),
                    j=0
       for -ms/2 <= k1 <= (ms-1)/2,
           -mt/2 <= k2 <= (mt-1)/2,  -mu/2 <= k3 <= (mu-1)/2
```

Parameters

- **x** (*float[nj]*) – nonuniform source x-coords, valid only in [-3pi,3pi]
- **y** (*float[nj]*) – nonuniform source y-coords, valid only in [-3pi,3pi]
- **z** (*float[nj]*) – nonuniform source z-coords, valid only in [-3pi,3pi]
- **c** (*complex[nj]*) – source strengths
- **isign** (*int*) – if >=0, uses + sign in exponential, otherwise - sign
- **eps** (*float*) – precision requested (>1e-16)
- **ms** (*int*) – number of Fourier modes in x-direction, may be even or odd; in either case the modes are integers lying in [-ms/2, (ms-1)/2]
- **mt** (*int*) – number of Fourier modes in y-direction, may be even or odd; in either case the modes are integers lying in [-mt/2, (mt-1)/2]
- **mu** (*int*) – number of Fourier modes in z-direction, may be even or odd; in either case the modes are integers lying in [-mu/2, (mu-1)/2]
- **f** (*complex[ms,mt,mu]*) – output Fourier mode values. Should be initialized as a Fortran-ordered (ie ms fastest) numpy array of the correct size
- **debug** (*int, optional*) – 0 (silent), 1 (print timing breakdown)
- **spread_debug** (*int, optional*) – 0 (silent), 1, 2... (prints spreader info)
- **spread_sort** (*int, optional*) – 0 (don't sort NU pts in spreader), 1 (sort)
- **fftw** (*int, optional*) – 0 (use FFTW_ESTIMATE), 1 (use FFTW_MEASURE)
- **modeord** (*int, optional*) – 0 (CMCL increasing mode ordering), 1 (FFT ordering)
- **chkbnds** (*int, optional*) – 0 (don't check NU points valid), 1 (do)

Note: The output is written into the f array.

Returns 0 if success, 1 if eps too small, 2 if size of arrays to malloc exceed MAX_NF, 4 at least one NU point out of range (if chkbnds true)

Return type int

Example

see `python_tests/accuracy_speed_tests.py`

`finufftpy.`**`nufft3d2`**(*x*, *y*, *z*, *c*, *isign*, *eps*, *f*, *debug=0*, *spread_debug=0*, *spread_sort=1*, *fftw=0*, *modeord=0*, *chkbnds=1*)

3D type-2 (aka forward) complex nonuniform fast Fourier transform

```
    c[j] =   SUM   f[k1,k2,k3] exp(+/-i (k1 x[j] + k2 y[j] + k3 z[j])).
           k1,k2,k3
                     for j = 0,...,nj-1,  where sum is over
    -ms/2 <= k1 <= (ms-1)/2, -mt/2 <= k2 <= (mt-1)/2, -mu/2 <= k3 <= (mu-1)/2
```

Parameters

- **x** (*float[nj]*) – nonuniform target x-coords, valid only in [-3pi,3pi]
- **y** (*float[nj]*) – nonuniform target y-coords, valid only in [-3pi,3pi]
- **z** (*float[nj]*) – nonuniform target z-coords, valid only in [-3pi,3pi]
- **c** (*complex[nj]*) – output values at targets. Should be initialized as a numpy array of the correct size
- **isign** (*int*) – if >=0, uses + sign in exponential, otherwise - sign
- **eps** (*float*) – precision requested (>1e-16)
- **f** (*complex[ms,mt,mu]*) – Fourier mode coefficients, where ms, mt and mu are either even or odd; in either case their mode range is integers lying in [-m/2, (m-1)/2], with mode ordering in all dimensions given by modeord. Ordering is Fortran-style, ie ms fastest.
- **debug** (*int, optional*) – 0 (silent), 1 (print timing breakdown)
- **spread_debug** (*int, optional*) – 0 (silent), 1, 2... (print spreader info)
- **spread_sort** (*int, optional*) – 0 (don't sort NU pts in spreader), 1 (sort)
- **fftw** (*int, optional*) – 0 (use FFTW_ESTIMATE), 1 (use FFTW_MEASURE)
- **modeord** (*int, optional*) – 0 (CMCL increasing mode ordering), 1 (FFT ordering)
- **chkbnds** (*int, optional*) – 0 (don't check NU points valid), 1 (do)

Note: The output is written into the c array.

Returns 0 if success, 1 if eps too small, 2 if size of arrays to malloc exceed MAX_NF, 4 at least one NU point out of range (if chkbnds true)

Return type int

Example

see `python_tests/accuracy_speed_tests.py`

finufftpy.**nufft3d3**(*x*, *y*, *z*, *c*, *isign*, *eps*, *s*, *t*, *u*, *f*, *debug=0*, *spread_debug=0*, *spread_sort=1*, *fftw=0*)
3D type-3 (NU-to-NU) complex nonuniform fast Fourier transform

```
            nj-1
f[k]   =    SUM   c[j] exp(+-i s[k] x[j] + t[k] y[j] + u[k] z[j]),
            j=0
                                                    for k = 0,...,nk-1
```

Parameters

- **x** (*float[nj]*) – nonuniform source point x-coords, in R
- **y** (*float[nj]*) – nonuniform source point y-coords, in R
- **z** (*float[nj]*) – nonuniform source point z-coords, in R
- **c** (*complex[nj]*) – source strengths
- **isign** (*int*) – if >=0, uses + sign in exponential, otherwise - sign
- **eps** (*float*) – precision requested (>1e-16)
- **s** (*float[nk]*) – nonuniform target x-frequencies, in R
- **t** (*float[nk]*) – nonuniform target y-frequencies, in R
- **u** (*float[nk]*) – nonuniform target z-frequencies, in R
- **f** (*complex[nk]*) – output values at target frequencies. Should be initialized as a numpy array of the correct size
- **debug** (*int, optional*) – 0 (silent), 1 (print timing breakdown)
- **spread_debug** (*int, optional*) – 0 (silent), 1, 2... (print spreader info)
- **spread_sort** (*int, optional*) – 0 (don't sort NU pts in spreader), 1 (sort)
- **fftw** (*int, optional*) – 0 (use FFTW_ESTIMATE), 1 (use FFTW_MEASURE)

Note: The output is written into the f array.

Returns 0 if success, 1 if eps too small, 2 if size of arrays to malloc exceed MAX_NF

Return type int

Example

see `python_tests/accuracy_speed_tests.py`

CHAPTER

SEVEN

KNOWN ISSUES

One should also check the github issues for the project page, https://github.com/ahbarnett/finufft/issues

MATLAB

A segfault occurs if MATLAB's `fft` is called before the first `finufft` call in a session. We believe this due to incompatibility between the versions of FFTW used. Please contact us if you know of a fix.

Workaround: in your `startup.m` file, include a dummy call as follows:

```
finufft1d1(1,1,1,1,1);
```

This issue does not occur with octave.

CHAPTER

EIGHT

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- Leslie Greengard and June-Yub Lee - CMCL fortran drivers and test codes
- Dan Foreman-Mackey - python wrappers
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- Andras Pataki - complex number speed in C++
- Marina Spivak - fortran testing
- Christian Muller - optimization (CMA-ES) for early kernel design
- Timo Heister - pass/fail numdiff testing ideas
- Hannah Lawrence - user testing and finding bugs
- Zydrunas Gimbutas - explanation that NFFT uses Kaiser-Bessel backwards
- David Stein - feature requests and python help
- Joakim Anden - catching memory leak
- Dylan Simon - sphinx help

CHAPTER

NINE

REFERENCES

References for this software and the underlying mathematics include:

[FIN] FINUFFT: a fast and lightweight nonuniform fast Fourier transform library. A. H. Barnett and J. F. Magland. In preparation (2017).

[ORZ] Prolate Spheroidal Wave Functions of Order Zero: Mathematical Tools for Bandlimited Approximation. A. Osipov, V. Rokhlin, and H. Xiao. Springer (2013).

[KK] Chapter 7. System Analysis By Digital Computer. F. Kuo and J. F. Kaiser. Wiley (1967).

[FS] Nonuniform fast Fourier transforms using min-max interpolation. J. A. Fessler and B. P. Sutton. IEEE Trans. Sig. Proc., 51(2):560-74, (Feb. 2003)

[KKP] Using NFFT3—a software library for various nonequispaced fast Fourier transforms. J. Keiner, S. Kunis and D. Potts. Trans. Math. Software 36(4) (2009).

[F] Non-equispaced fast Fourier transforms with applications to tomography. K. Fourmont. J. Fourier Anal. Appl. 9(5) 431-450 (2003).

This code builds upon the CMCL NUFFT, and the Fortran wrappers are very similar to its interfaces. For that the following are references:

[GL] Accelerating the Nonuniform Fast Fourier Transform. L. Greengard and J.-Y. Lee. SIAM Review 46, 443 (2004).

[LG] The type 3 nonuniform FFT and its applications. J.-Y. Lee and L. Greengard. J. Comput. Phys. 206, 1 (2005).

The original NUFFT analysis using truncated Gaussians is:

[DR] Fast Fourier Transforms for Nonequispaced data. A. Dutt and V. Rokhlin. SIAM J. Sci. Comput. 14, 1368 (1993).

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